

What is claimed is:

Claims

- 1 1. A method of characterizing a mixture of components, the method comprising the  
2 steps of:  
3 obtaining a plurality of spectrochromatograms of the mixture of components,  
4 each of the spectrochromatograms being obtained under a respective one of  
5 a plurality of different chromatographic conditions;  
6 estimating the number of components and  
7 performing component matching upon the spectrochromatograms using the  
8 estimated number of components.
- 1 2. The method of claim 1 further comprising the step of determining each  
2 component retention time in response to the component matching.
- 1 3. The method of claim 1 further comprising the step of determining each  
2 component spectral shape in response to the component matching.
- 1 4. The method of claim 3 further comprising the step of using the component  
2 spectral shape to identify the component.
- 1 5. The method of claim 1 further comprising the step of resolving at least one  
2 component in the mixture of components.
- 1 6. A method of component peak matching comprising the steps of:  
2 obtaining a plurality of spectrochromatographic data sets for a mixture of  
3 components, each spectrochromatographic data set comprising  
4 spectrochromatographic data;  
5 creating an augmented spectrochromatographic data set by merging the  
6 spectrochromatographic data sets into a matrix;  
7 determining a preliminary estimate of the number of components (n) in the  
8 augmented spectrochromatographic data set;  
9 selecting the (n) most orthogonal spectrochromatographic data from the  
10 augmented spectrochromatographic data set;  
11 generating a refined key spectra set; and

- 12 determining the component retention times.
- 1 7. The method of claim 6 further comprising the step of:  
2 validating each of the (n) most orthogonal spectrochromatographic data using  
3 target factor analysis to generate the refined key spectra set.
- 1 8. The method of claim 6 further comprising the step of detecting missing  
2 components using target testing of each spectrochromatographic data in the refined key  
3 spectra set against each of the plurality of spectrochromatographic data sets.
- 1 9. The method of claim 6 wherein the step of determining a preliminary estimate  
2 uses principle component analysis.
- 1 10. The method of claim 6 wherein the step of determining a preliminary estimate  
2 uses single value decomposition.
- 1 11. The method of claim 6 wherein the step of determining a preliminary estimate  
2 uses nonlinear iterative partial least squares.
- 1 12. The method of claim 6 wherein the step of selecting the (n) most orthogonal  
2 spectra uses modified Iterative Key Set Factor Analysis.
- 1 13. The method of claim 6 wherein the step of determining the component retention  
2 times comprises:  
3 performing a regression using the refined key spectra set and the augmented data  
4 matrix; and  
5 determining retention times as maximum values.
- 1 14. A method for resolving a mixed sample of chromatographic components, the  
2 method comprising the steps of:  
3 selecting a plurality of differing chromatographic conditions;  
4 performing a plurality of chromatographic runs on the mixed sample, each  
5 respective run performed under a respective chromatographic condition;  
6 obtaining spectrochromatographic data for the mixed sample during each of the  
7 chromatographic runs;  
8 creating an augmented data set from the spectrochromatographic data of the  
9 plurality of chromatographic runs;

10           operating on the augmented data set to determine the retention times for each  
11           component in the mixed sample; and  
12           resolving each of the components.

1   15.       The method of claim 14 further comprising the step of performing component  
2   quantitation.

1   16.       The method of claim 15 wherein the step of performing component  
2   quantitation uses resolved spectra and concentration profiles.

1   17.       The method of claim 14 further comprising the step of finding peak relative  
2   areas using concentration profiles.

1   18.       A method of obtaining the shape of components from spectrochromatographic  
2   data comprising the steps of:

3           determining the number of components (n) and each component's retention time;

4           generating uniqueness vectors as initial estimates of spectrochromatographic

5           profiles; and

6           performing profile resolution on the spectrochromatographic data.

1   19.       The method of claim 18 wherein the step of performing profile resolution uses  
2   ALS MCR.